

300

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal626gms

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 Apr 08 "Ask CAS" for self-help around the clock  
NEWS 3 Jun 03 New e-mail delivery for search results now available  
NEWS 4 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN  
NEWS 5 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)  
now available on STN  
NEWS 6 Aug 26 Sequence searching in REGISTRY enhanced  
NEWS 7 Sep 03 JAPIO has been reloaded and enhanced  
NEWS 8 Sep 16 Experimental properties added to the REGISTRY file  
NEWS 9 Sep 16 CA Section Thesaurus available in CAPLUS and CA  
NEWS 10 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985  
NEWS 11 Oct 24 BEILSTEIN adds new search fields  
NEWS 12 Oct 24 Nutraceuticals International (NUTRACEUT) now available on STN  
NEWS 13 Nov 18 DKILIT has been renamed APOLLIT  
NEWS 14 Nov 25 More calculated properties added to REGISTRY  
NEWS 15 Dec 04 CSA files on STN  
NEWS 16 Dec 17 PCTFULL now covers WP/PCT Applications from 1978 to date  
NEWS 17 Dec 17 TOXCENTER enhanced with additional content  
NEWS 18 Dec 17 Adis Clinical Trials Insight now available on STN  
NEWS 19 Jan 29 Simultaneous left and right truncation added to COMPENDEX,  
ENERGY, INSPEC  
NEWS 20 Feb 13 CANCERLIT is no longer being updated  
NEWS 21 Feb 24 METADEX enhancements  
NEWS 22 Feb 24 PCTGEN now available on STN  
NEWS 23 Feb 24 TEMA now available on STN  
NEWS 24 Feb 26 NTIS now allows simultaneous left and right truncation  
NEWS 25 Feb 26 PCTFULL now contains images  
NEWS 26 Mar 04 SDI PACKAGE for monthly delivery of multifile SDI results  
NEWS 27 Mar 19 APOLLIT offering free connect time in April 2003  
NEWS 28 Mar 20 EVENTLINE will be removed from STN  
NEWS 29 Mar 24 PATDPAFULL now available on STN  
NEWS 30 Mar 24 Additional information for trade-named substances without  
structures available in REGISTRY  
NEWS 31 Mar 24 Indexing from 1957 to 1966 added to records in CA/CAPLUS  
NEWS 32 Apr 11 Display formats in DGENE enhanced  
NEWS 33 Apr 14 MEDLINE Reload  
NEWS 34 Apr 17 Polymer searching in REGISTRY enhanced  
  
NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT  
MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),  
AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003  
  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items

Golam Shameem

NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 14:26:57 ON 18 APR 2003

=> FIL REGISTRY

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 14:27:05 ON 18 APR 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 17 APR 2003 HIGHEST RN 503414-07-1

DICTIONARY FILE UPDATES: 17 APR 2003 HIGHEST RN 503414-07-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

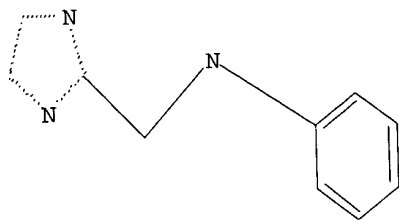
Uploading 10019976.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 14:27:29 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 698 TO ITERATE

100.0% PROCESSED 698 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

50 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 12376 TO 15544  
PROJECTED ANSWERS: 752 TO 1688

L2 50 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 14:27:36 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 13698 TO ITERATE

100.0% PROCESSED 13698 ITERATIONS  
SEARCH TIME: 00.00.02

1174 ANSWERS

L3 1174 SEA SSS FUL L1

=>

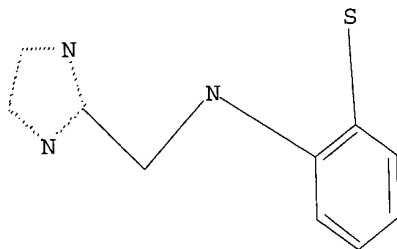
Uploading 10019976a.str

L4 STRUCTURE UPLOADED

=> d l4

L4 HAS NO ANSWERS

L4 STR



Structure attributes must be viewed using STN Express query preparation.

Golam Shameem

=> s l4

SAMPLE SEARCH INITIATED 14:29:49 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 15 TO ITERATE

100.0% PROCESSED 15 ITERATIONS  
SEARCH TIME: 00.00.01

4 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 68 TO 532  
PROJECTED ANSWERS: 4 TO 200

L5 4 SEA SSS SAM L4

=> s l4 sss full

FULL SEARCH INITIATED 14:29:57 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 330 TO ITERATE

100.0% PROCESSED 330 ITERATIONS  
SEARCH TIME: 00.00.01

56 ANSWERS

L6 56 SEA SSS FUL L4

=> FIL CAPLUS

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
297.50	297.71

FILE 'CAPLUS' ENTERED AT 14:30:15 ON 18 APR 2003  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE COVERS 1907 - 18 Apr 2003 VOL 138 ISS 17  
FILE LAST UPDATED: 17 Apr 2003 (20030417/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l6

L7

4 L6

=> d ibib abs hitster 17 tot

L7 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 2002:312317 CAPLUS

Golam Shameem

DOCUMENT NUMBER: 137:56986  
TITLE: 2-(Anilinomethyl)imidazolines as .alpha.1 Adrenergic Receptor Agonists: the Discovery of .alpha.1a Subtype Selective 2'-Alkylsulfonyl-Substituted Analogues  
AUTHOR(S): Hodson, Stephen J.; Bishop, Michael J.; Speake, Jason D.; Navas, Frank, III; Garrison, Deanna T.; Bigham, Eric C.; Saussy, David L., Jr.; Liacos, James A.; Irving, Paul E.; Gobel, M. Jeffrey; Sherman, Bryan W.  
CORPORATE SOURCE: GlaxoSmithKline Research Laboratories, Research Triangle Park, NC, 27709-3398, USA  
SOURCE: Journal of Medicinal Chemistry (2002), 45(11), 2229-2239  
CODEN: JMCMAR; ISSN: 0022-2623  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 137:56986

AB A series of 2'-alkylthio-2-(anilinomethyl)imidazolines were prepd. to examine the effect of the alkyl group size, sulfur oxidn. state, and Ph ring substitution on ligand binding and agonism of .alpha.-adrenergic receptor subtypes .alpha.1a, .alpha.1b, .alpha.1d, .alpha.2a, and .alpha.2c. Binding at all receptor subtypes decreased for compds. in the sulfone oxidn. state as compared to their sulfide analogs. While sulfides were generally potent, nonselective agonists, sulfones exhibited .alpha.1a subtype selectivity in a cell-based functional assay. One of the sulfones was 250-7000-fold selective for .alpha.1a vs. all other subtypes.

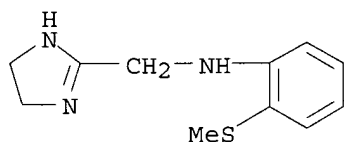
IT 67083-77-6P 439291-53-9P 439291-54-0P  
439291-56-2P 439291-59-5P 439291-62-0P  
439291-64-2P 439291-66-4P 439291-70-0P  
439291-72-2P 439291-74-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and structure activity relationships of 2-(anilinomethyl)imidazolines as .alpha.1 adrenergic receptor agonists)

RN 67083-77-6 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-(methylthio)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

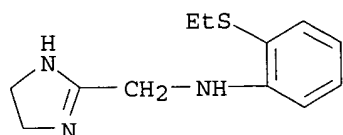
RN 439291-53-9 CAPLUS

CN 1H-Imidazole-2-methanamine, N-[2-(ethylthio)phenyl]-4,5-dihydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 439291-52-8

CMF C12 H17 N3 S

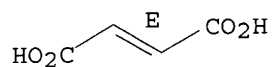


CM 2

CRN 110-17-8

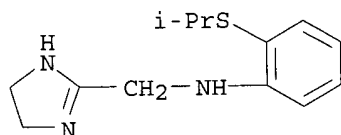
CMF C4 H4 O4

Double bond geometry as shown.



RN 439291-54-0 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-[(1-methylethyl)thio]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

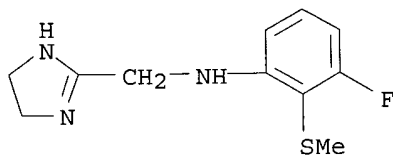
RN 439291-56-2 CAPLUS

CN 1H-Imidazole-2-methanamine, N-[3-fluoro-2-(methylthio)phenyl]-4,5-dihydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 439291-55-1

CMF C11 H14 F N3 S



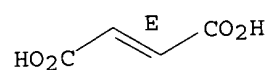
CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.

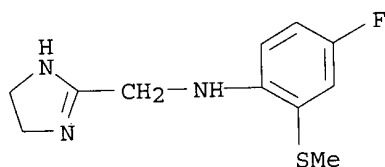
Golam Shameem



RN 439291-59-5 CAPLUS  
CN 1H-Imidazole-2-methanamine, N-[4-fluoro-2-(methylthio)phenyl]-4,5-dihydro-  
, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

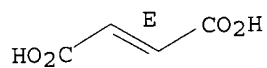
CRN 439291-58-4  
CMF C11 H14 F N3 S



CM 2

CRN 110-17-8  
CMF C4 H4 O4

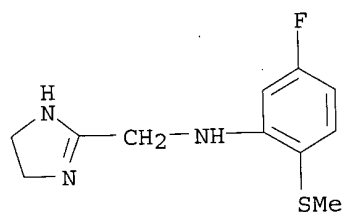
Double bond geometry as shown.



RN 439291-62-0 CAPLUS  
CN 1H-Imidazole-2-methanamine, N-[5-fluoro-2-(methylthio)phenyl]-4,5-dihydro-  
, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 439291-61-9  
CMF C11 H14 F N3 S

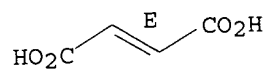


CM 2

CRN 110-17-8  
CMF C4 H4 O4

Golam Shameem

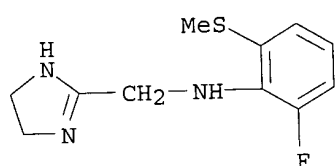
Double bond geometry as shown.



RN 439291-64-2 CAPLUS  
CN 1H-Imidazole-2-methanamine, N-[2-fluoro-6-(methylthio)phenyl]-4,5-dihydro-  
, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

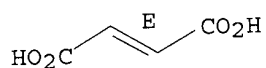
CRN 439291-63-1  
CMF C11 H14 F N3 S



CM 2

CRN 110-17-8  
CMF C4 H4 O4

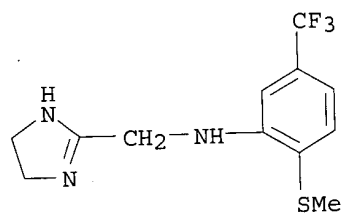
Double bond geometry as shown.



RN 439291-66-4 CAPLUS  
CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-(methylthio)-5-(trifluoromethyl)phenyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 439291-65-3  
CMF C12 H14 F3 N3 S



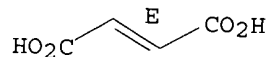
CM 2

Golam Shameem



CRN 110-17-8  
CMF C4 H4 O4

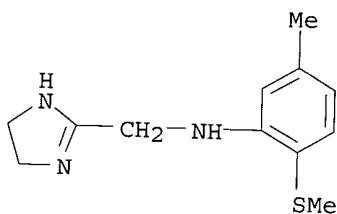
Double bond geometry as shown.



RN 439291-70-0 CAPLUS  
CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[5-methyl-2-(methylthio)phenyl]-  
, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

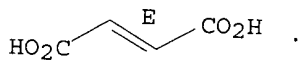
CRN 439291-69-7  
CMF C12 H17 N3 S



CM 2

CRN 110-17-8  
CMF C4 H4 O4

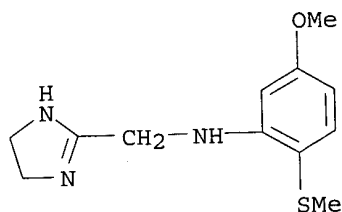
Double bond geometry as shown.



RN 439291-72-2 CAPLUS  
CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[5-methoxy-2-(methylthio)phenyl]-  
, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

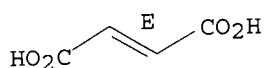
CRN 439291-71-1  
CMF C12 H17 N3 O S



CM 2

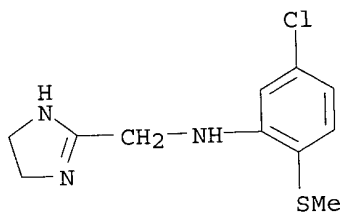
CRN 110-17-8  
CMF C4 H4 O4

Double bond geometry as shown.



RN 439291-74-4 CAPLUS  
CN 1H-Imidazole-2-methanamine, N-[5-chloro-2-(methylthio)phenyl]-4,5-dihydro-  
, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

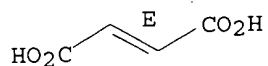
CM 1

CRN 439291-73-3  
CMF C11 H14 Cl N3 S

CM 2

CRN 110-17-8  
CMF C4 H4 O4

Double bond geometry as shown.



IT 305809-48-7P 305809-50-1P 305809-52-3P  
305809-54-5P 305809-55-6P 305809-57-8P  
305809-59-0P 305809-61-4P 305809-63-6P  
305809-64-7P 305811-04-5P 439291-51-7P  
439291-68-6P 439291-76-6P

Golam Shameem

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and structure activity relationships of 2-  
(anilinomethyl)imidazolines as .alpha.1 adrenergic receptor agonists)

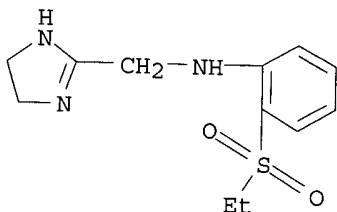
RN 305809-48-7 CAPLUS

CN 1H-Imidazole-2-methanamine, N-[2-(ethylsulfonyl)phenyl]-4,5-dihydro-,  
(2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-47-6

CMF C12 H17 N3 O2 S

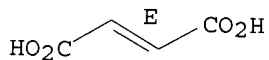


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



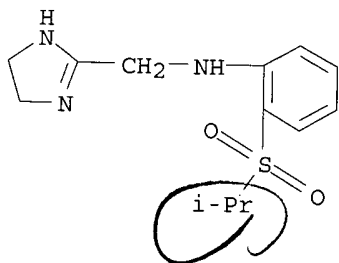
RN 305809-50-1 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-[(1-methylethyl)sulfonyl]phenyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-49-8

CMF C13 H19 N3 O2 S



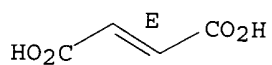
CM 2

CRN 110-17-8

*bad date*

CMF C4 H4 O4

Double bond geometry as shown.



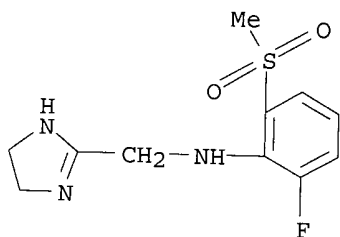
RN 305809-52-3 CAPLUS

CN 1H-Imidazole-2-methanamine, N-[2-fluoro-6-(methylsulfonyl)phenyl]-4,5-dihydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-51-2

CMF C11 H14 F N3 O2 S

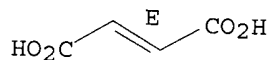


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



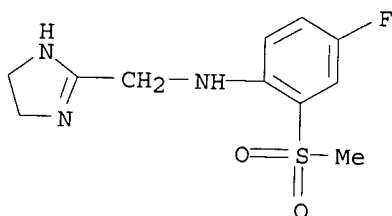
RN 305809-54-5 CAPLUS

CN 1H-Imidazole-2-methanamine, N-[4-fluoro-2-(methylsulfonyl)phenyl]-4,5-dihydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-53-4

CMF C11 H14 F N3 O2 S

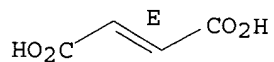


CM 2

CRN 110-17-8

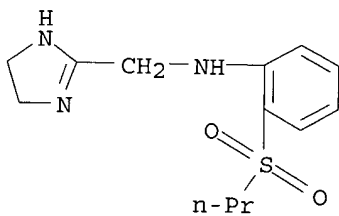
CMF C4 H4 O4

Double bond geometry as shown.



RN 305809-55-6 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-(propylsulfonyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

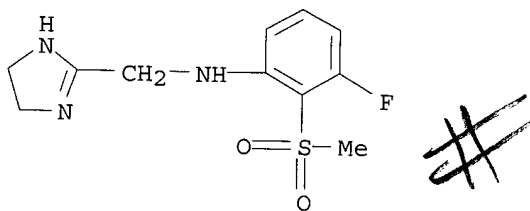
RN 305809-57-8 CAPLUS

CN 1H-Imidazole-2-methanamine, N-[3-fluoro-2-(methylsulfonyl)phenyl]-4,5-dihydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-56-7

CMF C11 H14 F N3 O2 S



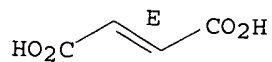
CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.

Golam Shameem



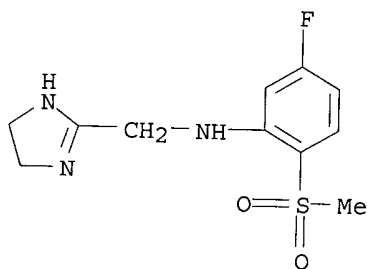
RN 305809-59-0 CAPLUS

CN 1H-Imidazole-2-methanamine, N-[5-fluoro-2-(methylsulfonyl)phenyl]-4,5-dihydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-58-9

CMF C11 H14 F N3 O2 S

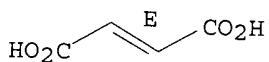


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



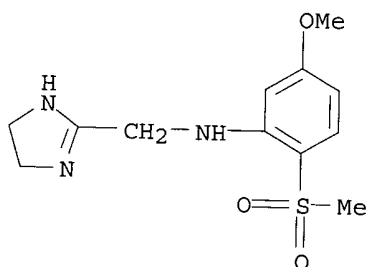
RN 305809-61-4 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[5-methoxy-2-(methylsulfonyl)phenyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-60-3

CMF C12 H17 N3 O3 S

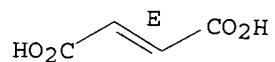


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



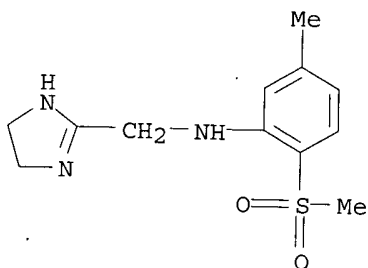
RN 305809-63-6 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[5-methyl-2-(methylsulfonyl)phenyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-62-5

CMF C12 H17 N3 O2 S

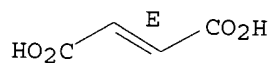


CM 2

CRN 110-17-8

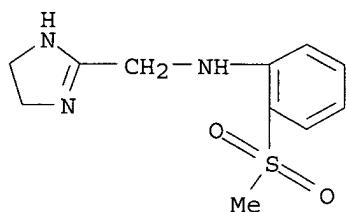
CMF C4 H4 O4

Double bond geometry as shown.



RN 305809-64-7 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-(methylsulfonyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

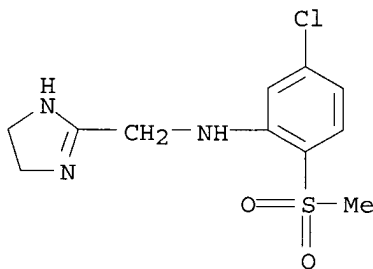


● HCl

RN 305811-04-5 CAPLUS  
CN 1H-Imidazole-2-methanamine, N-[5-chloro-2-(methylsulfonyl)phenyl]-4,5-dihydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

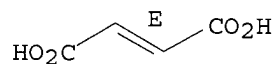
CRN 305811-03-4  
CMF C11 H14 Cl N3 O2 S



CM 2

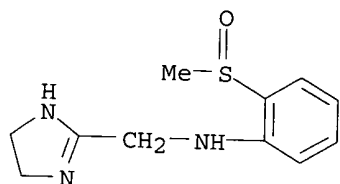
CRN 110-17-8  
CMF C4 H4 O4

Double bond geometry as shown.



RN 439291-51-7 CAPLUS  
CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-(methylsulfinyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



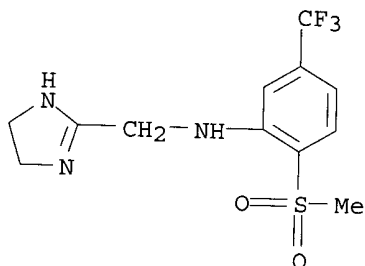


● HCl

RN 439291-68-6 CAPLUS  
 CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-(methylsulfonyl)-5-(trifluoromethyl)phenyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

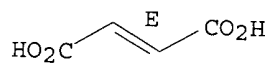
CRN 439291-67-5  
 CMF C12 H14 F3 N3 O2 S



CM 2

CRN 110-17-8  
 CMF C4 H4 O4

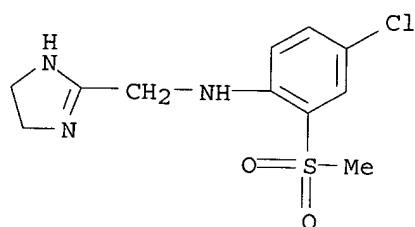
Double bond geometry as shown.



RN 439291-76-6 CAPLUS  
 CN 1H-Imidazole-2-methanamine, N-[4-chloro-2-(methylsulfonyl)phenyl]-4,5-dihydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 439291-75-5  
 CMF C11 H14 Cl N3 O2 S

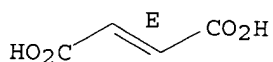


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:790481 CAPLUS

DOCUMENT NUMBER: 133:350215

TITLE: Arylaminoethylimidazolines as .alpha.1A adrenoceptor agonists

INVENTOR(S): Bigham, Eric; Cleveland; Bishop, Michael Joseph; Drewry, David Harold; Garrison, Deanna Trojan; Hodson, Stephen Joseph; Navas, Frank, III; Speake, Jason D.

PATENT ASSIGNEE(S): Glaxo Group Limited, UK; Navas Iii, Frank

SOURCE: PCT Int. Appl., 75 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

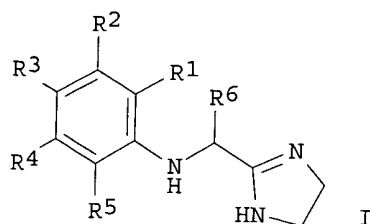
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066563	A1	20001109	WO 2000-EP3848	20000428
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
EP 1175406	A1	20020130	EP 2000-925251	20000428
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
JP 2002543187	T2	20021217	JP 2000-615394	20000428
PRIORITY APPLN. INFO.:			GB 1999-10110	A 19990430
			WO 2000-EP3848	W 20000428

OTHER SOURCE(S) :  
GI

MARPAT 133:350215



AB Title compds. I [R2-R5 = H, halogen, -OH, alkyl, alkoxy, alkylthio, CF<sub>3</sub>, .gtoreq. 2 of R2-R5 = H; R6 = H, Me; R1 = S(O)<sub>n</sub>R7 (n = 1, 2), SO<sub>2</sub>NHR8, COR9, NR10R11, CR12:NOR13, (un)substituted Ph, heterocyclic; R7, R8 = alkyl, fluoroalkyl; R9 = alkyl, fluoroalkyl, (un)substituted NH<sub>2</sub>, NHH2; R10 = H, alkyl; R11 = cycloalkyl, cyclopropylmethyl, alkenyl, (un)substituted alkyl; R12 = H, alkyl; R13 = alkyl] were prepd. for use in the treatment of .alpha.1A-mediated diseases or conditions such as urinary incontinence. Thus, 2-MeSC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> was treated with 2-chloromethyl-2-imidazoline-HCl and oxidized to give I [R1 = SO<sub>2</sub>Me, R2-R6 = H] as the fumarate, which was active as an agonist for cloned human .alpha.1A receptors.

IT 305809-66-9P 305809-68-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of arylaminomethylimidazolines as .alpha.1A adrenoceptor agonists)

RN 305809-66-9 CAPLUS

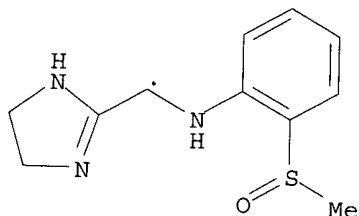
CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-(methylsulfinyl)phenyl]-, (-)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-65-8

CMF C11 H15 N3 O S

Rotation (-).

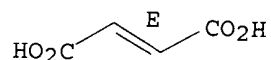


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



RN 305809-68-1 CAPLUS

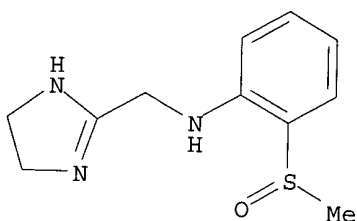
CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-(methylsulfinyl)phenyl]-, (+)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-67-0

CMF C11 H15 N3 O S

Rotation (+).

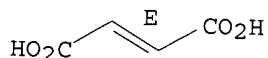


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



IT 305809-46-5P 305809-48-7P 305809-50-1P  
305809-52-3P 305809-54-5P 305809-55-6P  
305809-57-8P 305809-59-0P 305809-61-4P  
305809-63-6P 305809-64-7P 305810-08-6P  
305810-10-0P 305811-04-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of arylaminomethylimidazolines as .alpha.1A adrenoceptor agonists)

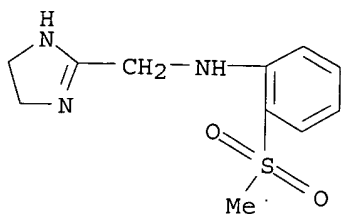
RN 305809-46-5 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-(methylsulfonyl)phenyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-45-4

CMF C11 H15 N3 O2 S

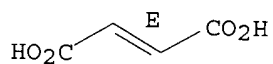


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



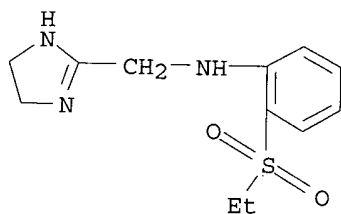
RN 305809-48-7 CAPLUS

CN 1H-Imidazole-2-methanamine, N-[2-(ethylsulfonyl)phenyl]-4,5-dihydro-,  
(2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-47-6

CMF C12 H17 N3 O2 S

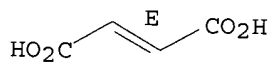


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



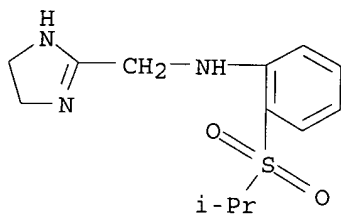
RN 305809-50-1 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-[(1-methylethyl)sulfonyl]phenyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-49-8

CMF C13 H19 N3 O2 S

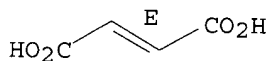


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



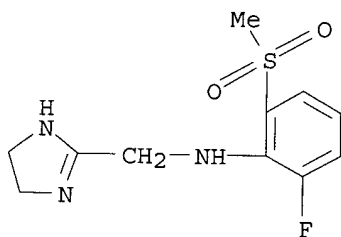
RN 305809-52-3 CAPLUS

CN 1H-Imidazole-2-methanamine, N-[2-fluoro-6-(methylsulfonyl)phenyl]-4,5-dihydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-51-2

CMF C11 H14 F N3 O2 S

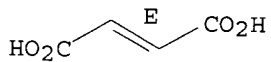


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.

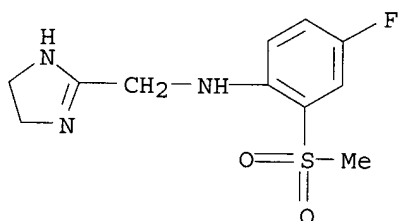


Golam Shameem

RN 305809-54-5 CAPLUS  
CN 1H-Imidazole-2-methanamine, N-[4-fluoro-2-(methylsulfonyl)phenyl]-4,5-dihydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

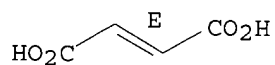
CRN 305809-53-4  
CMF C11 H14 F N3 O2 S



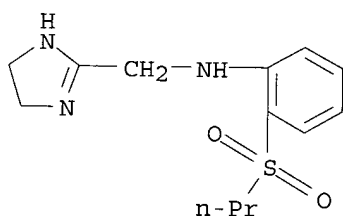
CM 2

CRN 110-17-8  
CMF C4 H4 O4

Double bond geometry as shown.



RN 305809-55-6 CAPLUS  
CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-(propylsulfonyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

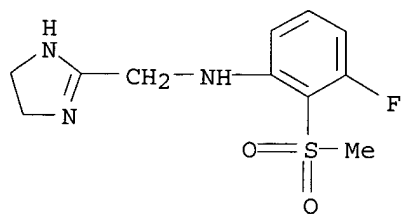


● HCl

RN 305809-57-8 CAPLUS  
CN 1H-Imidazole-2-methanamine, N-[3-fluoro-2-(methylsulfonyl)phenyl]-4,5-dihydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-56-7  
CMF C11 H14 F N3 O2 S

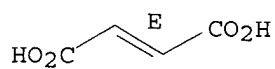


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



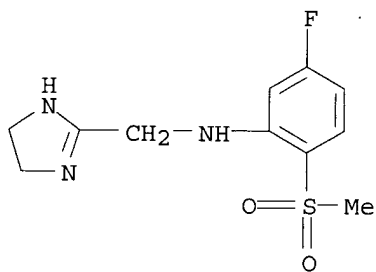
RN 305809-59-0 CAPLUS

CN 1H-Imidazole-2-methanamine, N-[5-fluoro-2-(methylsulfonyl)phenyl]-4,5-dihydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-58-9

CMF C11 H14 F N3 O2 S

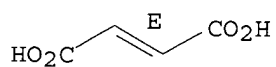


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



RN 305809-61-4 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[5-methoxy-2-

Golam Shameem

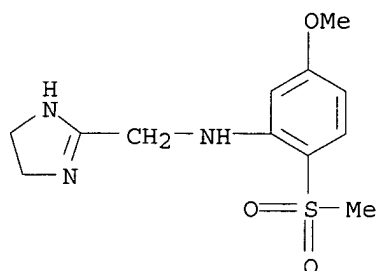


(methylsulfonyl)phenyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-60-3

CMF C12 H17 N3 O3 S

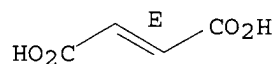


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



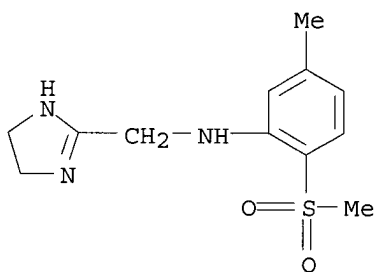
RN 305809-63-6 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[5-methyl-2-(methylsulfonyl)phenyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-62-5

CMF C12 H17 N3 O2 S

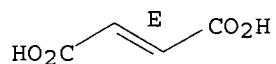


CM 2

CRN 110-17-8

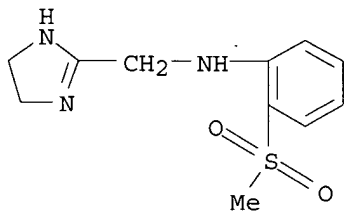
CMF C4 H4 O4

Double bond geometry as shown.



RN 305809-64-7 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-(methylsulfonyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

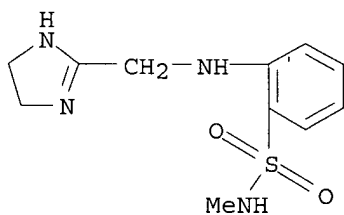
RN 305810-08-6 CAPLUS

CN Benzenesulfonamide, 2-[[[4,5-dihydro-1H-imidazol-2-yl)methyl]amino]-N-methyl-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305810-07-5

CMF C11 H16 N4 O2 S

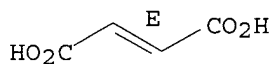


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



RN 305810-10-0 CAPLUS

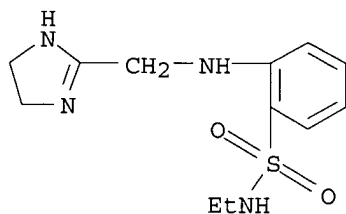
CN Benzenesulfonamide, 2-[[[4,5-dihydro-1H-imidazol-2-yl)methyl]amino]-N-ethyl-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

Golam Shameem

CM 1

CRN 305810-09-7

CMF C12 H18 N4 O2 S

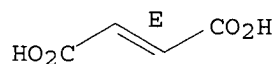


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



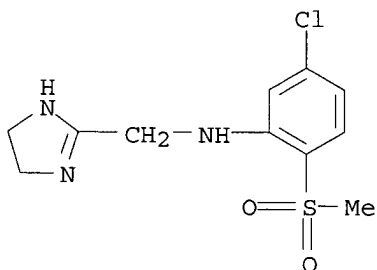
RN 305811-04-5 CAPLUS

CN 1H-Imidazole-2-methanamine, N-[5-chloro-2-(methylsulfonyl)phenyl]-4,5-dihydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305811-03-4

CMF C11 H14 Cl N3 O2 S

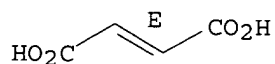


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.

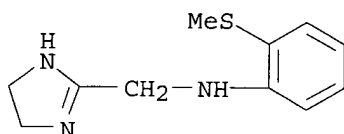


IT 305811-05-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. of arylaminomethylimidazolines as .alpha.1A adrenoceptor agonists)

RN 305811-05-6 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-(methylthio)phenyl]- (9CI)  
(CA INDEX NAME)



IT 305809-45-4P 305809-47-6P 305809-58-9P

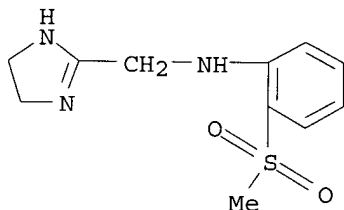
305809-60-3P 305809-62-5P 305810-07-5P

305810-09-7P 305811-03-4P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of arylaminomethylimidazolines as .alpha.1A adrenoceptor agonists)

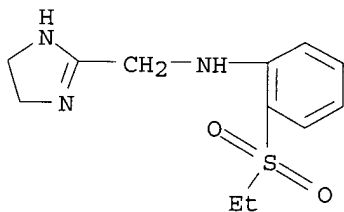
RN 305809-45-4 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



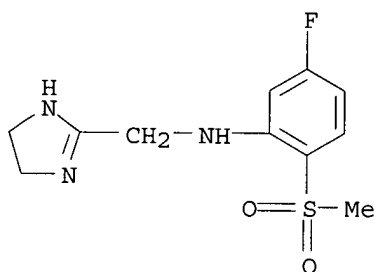
RN 305809-47-6 CAPLUS

CN 1H-Imidazole-2-methanamine, N-[2-(ethylsulfonyl)phenyl]-4,5-dihydro- (9CI)  
(CA INDEX NAME)



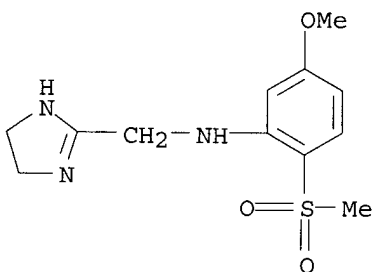
RN 305809-58-9 CAPLUS

CN 1H-Imidazole-2-methanamine, N-[5-fluoro-2-(methylsulfonyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



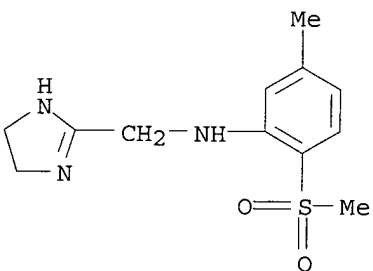
RN 305809-60-3 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[5-methoxy-2-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



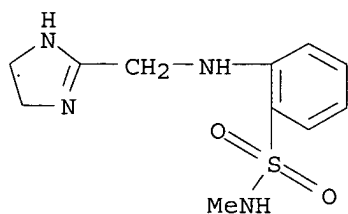
RN 305809-62-5 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[5-methyl-2-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



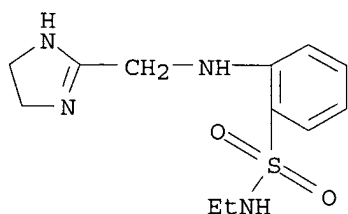
RN 305810-07-5 CAPLUS

CN Benzenesulfonamide, 2-[[[4,5-dihydro-1H-imidazol-2-yl)methyl]amino]-N-methyl- (9CI) (CA INDEX NAME)



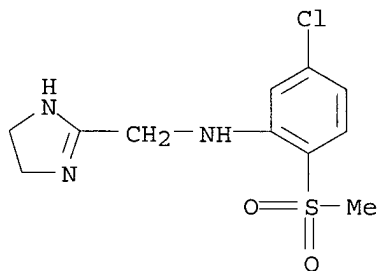
RN 305810-09-7 CAPLUS

CN Benzenesulfonamide, 2-[[4,5-dihydro-1H-imidazol-2-yl)methyl]amino]-N-ethyl- (9CI) (CA INDEX NAME)



RN 305811-03-4 CAPLUS

CN 1H-Imidazole-2-methanamine, N-[5-chloro-2-(methylsulfonyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1982:81362 CAPLUS

DOCUMENT NUMBER: 96:81362

TITLE: Imidazoline derivatives and their pesticidal use

INVENTOR(S): Kristinsson, Haukur; Traber, Walter

PATENT ASSIGNEE(S): Ciba-Geigy A.-G. , Switz.

SOURCE: Can., 29 pp. Division of Can. Appl. No. 290,708.

CODEN: CAXXA4

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

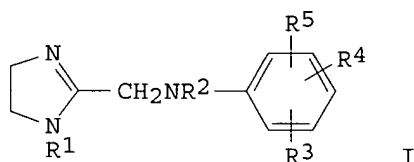
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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CA 1109787	A2	19810929	CA 1980-356272	19800715
CH 630507	A	19820630	CH 1977-12390	19771011
BE 860781	A1	19780516	BE 1977-182582	19771114
CA 1104143	A1	19810630	CA 1977-290708	19771114
ZA 7706801	A	19780927	ZA 1977-6801	19771115
CS 194822	P	19791231	CS 1977-7520	19771115

PRIORITY APPLN. INFO.:

CH 1976-14401	19761116
CH 1976-14402	19761116
CH 1977-12390	19771011
CA 1977-290708	19771114

GI



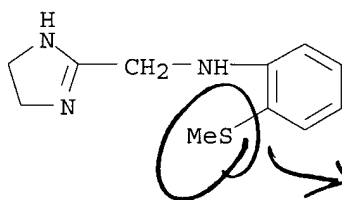
AB Hydrochlorides and free bases of anilinomethylimidazolines I (where R1 = H or alkyl; R2 = H, Me, pentyl, Bu, or substituted Ph; R3 = H, halo, Me, MeO, etc; R4 = R5 = H, halo, or Me) are pesticides. Thus, compns. contg. 2-(2'-methyl-3'-chlorophenylaminomethyl)-2-imidazoline (II) [80548-49-8] or an acid addn. salt with an inorg. or org. acid, together with a liq. or solid carrier or additive are suitable for ectoparasite control. Contact application of II HCl [67084-18-8] to engorged Boophilus microplus females resulted in 100% inhibition of oviposition at a min. concn. of 100 ppm in lab. tests. Syntheses of these imidazoline derivs. are described.

IT 67083-77-6P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. and pesticidal activity of)

RN 67083-77-6 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-(methylthio)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L7 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1978:541911 CAPLUS

DOCUMENT NUMBER: 89:141911

TITLE: Pesticidal composition for combatting ectoparasites and microorganisms

INVENTOR(S): Kristinsson, Haukur; Traber, Walter

Golam Shameem

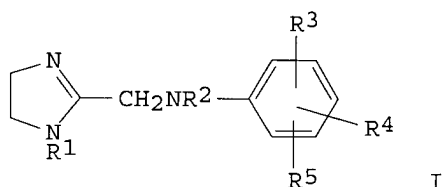
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.  
 SOURCE: Ger. Offen., 35 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2750902	A1	19780524	DE 1977-2750902	19771114
CH 630507	A	19820630	CH 1977-12390	19771011
NL 7712401	A	19780518	NL 1977-12401	19771110
BR 7707589	A	19780620	BR 1977-7589	19771111
BE 860781	A1	19780516	BE 1977-182582	19771114
GB 1592699	A	19810708	GB 1977-47367	19771114
IL 53374	A1	19830615	IL 1977-53374	19771114
ZA 7706801	A	19780927	ZA 1977-6801	19771115
ES 464150	A1	19790101	ES 1977-464150	19771115
AU 7730654	A1	19790524	AU 1977-30654	19771115
AU 526754	B2	19830127		
CS 194822	P	19791231	CS 1977-7520	19771115
JP 53063378	A2	19780606	JP 1977-137762	19771116
FR 2380733	A1	19780915	FR 1977-34431	19771116
FR 2380733	B1	19820730		
FR 2381030	A1	19780915	FR 1978-16218	19780531
FR 2381030	B1	19821001		

PRIORITY APPLN. INFO.:

CH 1976-14401 19761116  
 CH 1976-14402 19761116  
 CH 1977-12390 19771011

GI



AB The 2-phenylaminomethyl-2-imidazolines I (R1 = H or C1-10 alkyl; R2 = H, C1-10 alkyl or substituted Ph; R3, R4, and R5 = H, C1-5 alkyl, C1-5 alkoxy, alkylthio, OH, halo, NO2, CN, or CF3; R3R4 = 1,4-butadienyl) are acaricides and fungicides. Thus, the LC100 of 2-(2,3-dimethylphenylaminomethyl)-2-imidazoline-HCl (II) [67084-33-7] for *Ablyomma hebraeum* was 1 ppm. The synthesis of I is given. II was prepd. by the reaction of 2-chloromethyl-2-imidazoline-HCl [13338-49-3] with 2,3-dimethylaniline [87-59-2].

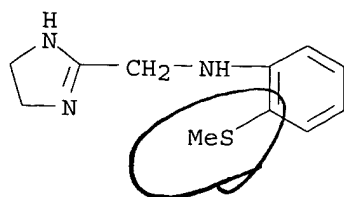
IT 67083-77-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and acaricidal and fungicidal activity of)

RN 67083-77-6 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-(methylthio)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)





● HCl

=> FIL REGISTRY

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
22.31	320.02

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-2.60	-2.60

CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 14:36:09 ON 18 APR 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 17 APR 2003 HIGHEST RN 503414-07-1

DICTIONARY FILE UPDATES: 17 APR 2003 HIGHEST RN 503414-07-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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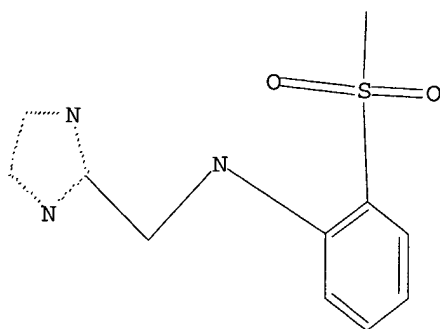
Uploading 10019976b.str

L8 STRUCTURE UPLOADED

=> d l8

L8 HAS NO ANSWERS

L8 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l8

SAMPLE SEARCH INITIATED 14:36:36 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 2 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 2 TO 124  
 PROJECTED ANSWERS: 2 TO 124

L9 2 SEA SSS SAM L8

=> FIL CAPLUS

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.40	320.42
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-2.60

FILE 'CAPLUS' ENTERED AT 14:36:41 ON 18 APR 2003  
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FILE COVERS 1907 - 18 Apr 2003 VOL 138 ISS 17  
 FILE LAST UPDATED: 17 Apr 2003 (20030417/ED)

Golam Shameem

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 14:26:57 ON 18 APR 2003)

FILE 'REGISTRY' ENTERED AT 14:27:05 ON 18 APR 2003

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L2 50 S L1

L3 1174 S L1 SSS FULL

L4 STRUCTURE UPLOADED

L5 4 S L4

L6 56 S L4 SSS FULL

FILE 'CAPLUS' ENTERED AT 14:30:15 ON 18 APR 2003

L7 4 S L6

FILE 'REGISTRY' ENTERED AT 14:36:09 ON 18 APR 2003

L8 STRUCTURE UPLOADED

L9 2 S L8

FILE 'CAPLUS' ENTERED AT 14:36:41 ON 18 APR 2003

=> s l8

**REGISTRY INITIATED**

Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 14:36:50 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 2 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 2 TO 124  
PROJECTED ANSWERS: 2 TO 124

L10 2 SEA SSS SAM L8

L11 2 L10

=> d ibib abs hitstr l11 tot

L11 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 2002:312317 CAPLUS  
DOCUMENT NUMBER: 137:56986  
TITLE: 2-(Anilinomethyl)imidazolines as .alpha.1 Adrenergic  
Receptor Agonists: the Discovery of .alpha.1a Subtype  
Selective 2'-Alkylsulfonyl-Substituted Analogues

AUTHOR(S): Hodson, Stephen J.; Bishop, Michael J.; Speake, Jason D.; Navas, Frank, III; Garrison, Deanna T.; Bigham, Eric C.; Saussy, David L., Jr.; Liacos, James A.; Irving, Paul E.; Gobel, M. Jeffrey; Sherman, Bryan W.

CORPORATE SOURCE: GlaxoSmithKline Research Laboratories, Research Triangle Park, NC, 27709-3398, USA

SOURCE: Journal of Medicinal Chemistry (2002), 45(11), 2229-2239

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:56986

AB A series of 2'-alkylthio-2-(anilinomethyl)imidazolines were prepd. to examine the effect of the alkyl group size, sulfur oxidn. state, and Ph ring substitution on ligand binding and agonism of .alpha.-adrenergic receptor subtypes .alpha.1a, .alpha.1b, .alpha.1d, .alpha.2a, and .alpha.2c. Binding at all receptor subtypes decreased for compds. in the sulfone oxidn. state as compared to their sulfide analogs. While sulfides were generally potent, nonselective agonists, sulfones exhibited .alpha.1a subtype selectivity in a cell-based functional assay. One of the sulfones was 250-7000-fold selective for .alpha.1a vs. all other subtypes.

IT 305809-50-1P 305809-59-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and structure activity relationships of 2-(anilinomethyl)imidazolines as .alpha.1 adrenergic receptor agonists)

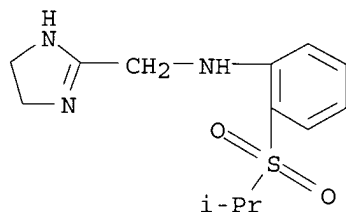
RN 305809-50-1 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-[(1-methylethyl)sulfonyl]phenyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

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CRN 305809-49-8

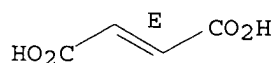
CMF C13 H19 N3 O2 S



CM 2

CRN 110-17-8  
CMF C4 H4 O4

Double bond geometry as shown.



RN 305809-59-0 CAPLUS

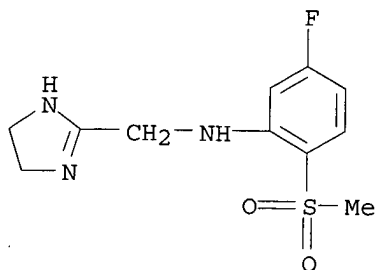
Golam Shameem

CN 1H-Imidazole-2-methanamine, N-[5-fluoro-2-(methylsulfonyl)phenyl]-4,5-dihydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-58-9

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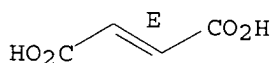


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



REFERENCE COUNT:

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THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:790481 CAPLUS

DOCUMENT NUMBER: 133-1350215

TITLE: Arylaminoethylimidazolines as  $\alpha_1A$  adrenoceptor agonists

INVENTOR(S) : Bigham, Eric Cleveland; Bishop, Michael Joseph;  
Drewry, David Harold; Garrison, Deanna Trojan; Hodson,  
Stephen Joseph; Navas, Frank, III; Speake, Jason D.

PATENT ASSIGNEE(S): ~~Stephen Cohen, Navas, Frank, III, Speake~~  
Glaxo Group Limited, UK; Navas III, Frank

SOURCE: PCT Int. Appl., 75 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

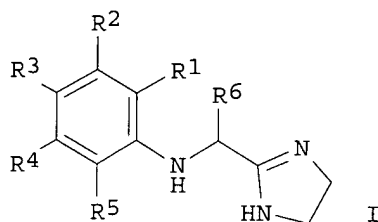
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066563	A1	20001109	WO 2000-EP3848	20000428

W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CR,
	CU,	CZ,	DE,	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,
	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	LU,
	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,
	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VN,	YU,	ZA,

ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,  
 DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,  
 CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
 EP 1175406 A1 20020130 EP 2000-925251 20000428  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO  
 JP 2002543187 T2 20021217 JP 2000-615394 20000428  
 PRIORITY APPLN. INFO.: GB 1999-10110 A 19990430  
 WO 2000-EP3848 W 20000428  
 OTHER SOURCE(S): MARPAT 133:350215  
 GI



AB Title compds. I [R2-R5 = H, halogen, -OH, alkyl, alkoxy, alkylthio, CF3, .gtoreq. 2 of R2-R5 = H; R6 = H, Me; R1 = S(O)nR7 (n = 1, 2), SO2NHR8, COR9, NR10R11, CR12:NOR13, (un)substituted Ph, heterocyclic; R7, R8 = alkyl, fluoroalkyl; R9 = alkyl, fluoroalkyl, (un)substituted NH2, NHHN2; R10 = H, alkyl; R11 = cycloalkyl, cyclopropylmethyl, alkenyl, (un)substituted alkyl; R12 = H, alkyl; R13 = alkyl] were prepd. for use in the treatment of .alpha.1A-mediated diseases or conditions such as urinary incontinence. Thus, 2-MeSC6H4NH2 was treated with 2-chloromethyl-2-imidazoline-HCl and oxidized to give I [R1 = SO2Me, R2-R6 = H] as the fumarate, which was active as an agonist for cloned human .alpha.1A receptors.

IT **305809-50-1P 305809-59-0P**  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of arylaminomethylimidazolines as .alpha.1A adrenoceptor agonists)

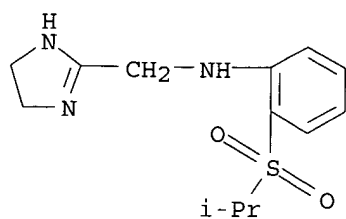
RN 305809-50-1 CAPLUS

CN 1H-Imidazole-2-methanamine, 4,5-dihydro-N-[2-[(1-methylethyl)sulfonyl]phenyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-49-8

CMF C13 H19 N3 O2 S

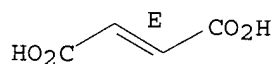


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



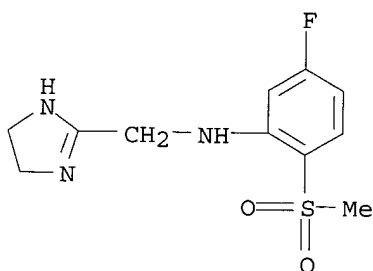
RN 305809-59-0 CAPLUS

CN 1H-Imidazole-2-methanamine, N-[5-fluoro-2-(methylsulfonyl)phenyl]-4,5-dihydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 305809-58-9

CMF C11 H14 F N3 O2 S

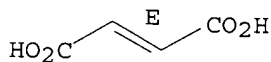


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

9.91

331.15

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-1.30

-3.90

STN INTERNATIONAL LOGOFF AT 14:38:00 ON 18 APR 2003